

Density Functional Theory for non-relativistic Fermions in the Unitarity Limit

Gautam Rupak^{*} and Thomas Schäfer[†]

Department of Physics, North Carolina State University, Raleigh, NC 27695

Abstract

We derive an energy density functional for non-relativistic spin one-half fermions in the limit of a divergent two-body scattering length. Using an epsilon expansion around $d = 4 - \epsilon$ spatial dimensions we compute the coefficient of the leading correction beyond the local density approximation (LDA). In the case of N fermionic atoms trapped in a harmonic potential this correction has the form $E = E_{LDA}(1 + c_s(3N)^{-2/3})$, where E_{LDA} is the total energy in LDA approximation. At next-to-leading order in the epsilon expansion we find $c_s = 1.68$, which is significantly larger than the result for non-interacting fermions, $c_s = 0.5$.

^{*} present address: Department of Physics and Astronomy, Mississippi State University, Mississippi State, MS 39762.
email: grupak@gmail.com

[†] email: thomas_schaefer@ncsu.edu

I. INTRODUCTION

Density functional theory (DFT) [1, 2] is widely used in condensed matter physics and quantum chemistry to treat quantum many-body systems. DFT relies on the fact that one can demonstrate the existence of an energy functional that depends only on the fermion density, and not on the wave functions, that has the property that the ground state energy can be obtained by minimizing the functional with respect to the density. There is renewed interest among nuclear theorists in developing a “Universal Nuclear Energy Density Functional” [3] which describes nuclear properties all across the isotopic chart, including very neutron rich nuclei far from the valley of stability. Ideally, this functional should be derived from a systematic theory of the nucleon-nucleon interaction. A modern approach to nuclear forces is provided by the effective field theory (EFT) method [4, 5, 6, 7]. EFT starts from the most general local lagrangian containing nucleon and pion fields that respects the basic symmetries of QCD. A power counting scheme determines the number of terms in the lagrangian, as well as the number of diagrams, that have to be kept at any given order in a low energy expansion.

If the effective field theory is perturbative then there are systematic methods for determining the energy density functional [8, 9]. However these methods are very cumbersome if long-range forces, such as pion exchange or collective modes, are important. In the case of non-perturbative EFT’s no systematic calculations of the energy density functional exist. In nuclear matter, and in cold fermionic gases near a Feshbach resonance, an important source of non-perturbative physics is the large two-body scattering length.

In the present work we try to address some of these problems by studying the energy density functional for a dilute system of non-relativistic spin 1/2 fermions with an infinite two-body scattering length. Because the s-wave cross section saturates the unitarity bound this limit is often referred to as the “unitarity limit”. The energy density functional in this limit is important for the study of neutron star crusts and neutron halos in nuclei. It can also be used to describe trapped fermionic atoms in the vicinity of a Feshbach resonance. The Fermi gas in the unitarity limit exhibits a number of interesting non-perturbative phenomena. It is a superfluid, and the ratio of the gap over the Fermi energy is large. Superfluidity implies that the $U(1)$ phase symmetry is spontaneously broken and the low energy or momentum response is carried by Goldstone modes.

We shall compute the energy density functional up to next-to-leading order (NLO) in an expansion in derivatives of the density. Our procedure is based on an effective lagrangian for the Fermi

gas in the unitarity limit derived in [10]. We will determine the coefficients in this lagrangian using an epsilon expansion around $d = 4 - \epsilon$ spatial dimensions [11, 12]. As a by-product we compute the phonon dispersion relation and the static susceptibility at NLO in the epsilon expansion. Our result for the energy density functional is rigorous when applied to infinite systems in which the density varies smoothly, but there are some limitations in the case of finite systems with a sharp surface, such as fermions confined in a harmonic trap. Pairing leads to an odd-even effect in the dependence of the energy on the number of particles, which a local energy density functional that depends only on the particle density cannot describe. Also, the gradient expansion breaks down near the surface of the system and the expansion of the energy in inverse fractional powers of the number of particles cannot be pushed to arbitrarily high order [10]. We shall discuss some possible approaches to overcome these limitations in Sec. V.

II. EFFECTIVE LAGRANGIAN AND ENERGY DENSITY FUNCTIONAL

The energy density functional describes the response of the system to smooth variations in the density. This functional can be related to the effective lagrangian that governs the response to slowly varying external fields. The effective Lagrangian at NLO in derivatives of the external potential is [10]

$$\mathcal{L} = c_0 m^{3/2} X^{5/2} + c_1 m^{1/2} \frac{(\vec{\nabla} X)^2}{\sqrt{X}} + \frac{c_2}{\sqrt{m}} \left[(\nabla^2 \phi)^2 - 9m \nabla^2 V \right] \sqrt{X}, \quad (1)$$

where we have defined

$$X = \mu - V - \phi - \frac{(\vec{\nabla} \phi)^2}{2m}. \quad (2)$$

The lagrangian contains the Goldstone boson (phonon) field $\phi(\vec{x}, t)$, the chemical potential μ , and the external potential $V(\vec{x}, t)$. The mass of the fermion is denoted by m . The functional form of the effective lagrangian is fixed by the symmetries of the problem, Galilean invariance, $U(1)$ symmetry, and conformal symmetry. The NLO effective lagrangian is characterized by three dimensionless parameters, c_0, c_1, c_2 . These parameters can be related to physical properties of the system. The first parameter, c_0 , can be related to the equation of state. We have

$$c_0 = \frac{2^{5/2}}{15\pi^2 \xi^{3/2}}, \quad (3)$$

where ξ determines the chemical potential in units of the Fermi energy, $\mu = \xi \epsilon_F$ with $\epsilon_F = k_F^2/(2m)$. The two NLO parameters c_1, c_2 are related to the momentum dependence of correla-

tion functions. The phonon dispersion relation, for example, is given by [10]

$$q_0 = v_s q \left[1 - \pi^2 \sqrt{2\xi} \left(c_1 + \frac{3}{2} c_2 \right) \frac{q^2}{k_F^2} + O(q^4 \log(q^2)) \right] \quad (4)$$

where $v_s = \sqrt{\xi/3} v_F$ is the speed of sound and $v_F = k_F/m$ is the Fermi velocity. The static susceptibility is defined by

$$\chi(q) = -i \int dt d^3x e^{-i\vec{q} \cdot \vec{x}} \langle \Psi^\dagger \Psi(0) \Psi^\dagger \Psi(t, \vec{x}) \rangle, \quad (5)$$

where $\Psi^\dagger \Psi \equiv \Psi_\alpha^\dagger \Psi^\alpha$ ($\alpha = 1, 2$) is the sum of the spin up and down densities. The susceptibility is related to a different linear combination of c_1 and c_2 [10],

$$\chi(q) = -\frac{mk_F}{\pi^2 \xi} \left[1 + 2\pi^2 \sqrt{2\xi} \left(c_1 - \frac{9}{2} c_2 \right) \frac{q^2}{k_F^2} + O(q^4 \log(q^2)) \right]. \quad (6)$$

The effective lagrangian can be used to compute the groundstate energy of fermions confined by an external potential. The energy of N fermions in a spherically symmetric trap $V(x) = \frac{1}{2} m \omega^2 x^2$ is

$$E = \frac{\sqrt{\xi}}{4} \omega (3N)^{4/3} - 3\sqrt{2}\pi^2 \xi \omega \left(c_1 - \frac{9}{2} c_2 \right) (3N)^{2/3} + \dots \quad (7)$$

In this work we will derive an energy functional that depends on the local density $n(x)$. This functional is the Legendre transform of the pressure,

$$\mathcal{E}[n(x)] = \mu n(x) - P[\mu - V(x)]. \quad (8)$$

The energy functional is easily derived from the effective lagrangian. Up to NLO in the derivative expansion it is sufficient to consider the tree-level effective lagrangian [10]. The only difficulty is to invert the relationship between the density and the chemical potential. This can be done order by order in the derivative expansion. We write

$$n[\mu - V(x)] = n_0[\mu - V(x)] + \delta n_1[\mu - V(x)] + \delta^2 n_2[\mu - V(x)] + \dots \quad (9)$$

$$\mu - V(x) = \mu_0[n(x)] + \delta \mu_1[n(x)] + \delta^2 \mu_2[n(x)] + \dots \quad (10)$$

$$\mathcal{E}[n(x)] = \mathcal{E}_0[n(x)] + \delta \mathcal{E}_1[n(x)] + \delta^2 \mathcal{E}_2[n(x)] + \dots, \quad (11)$$

where δ is used as an expansion parameter. The functions n_0, n_1, \dots arise from differentiating the leading order, next-to-leading, etc. terms in the effective lagrangian with respect to μ . The functions μ_0, μ_1, \dots can be found by inverting this relationship order by order. We find

$$\mathcal{E}_0[n(x)] = n(x)V(x) + \mu_0[n(x)]n(x) - P_0[\mu_0[n(x)]], \quad (12)$$

with $\mu_0[n(x)] = (n_0)^{-1}[n(x)]$ and $\mathcal{E}_1[n(x)] = -P_1(\mu_0[n(x)])$. This yields

$$\mathcal{E}(x) = n(x)V(x) + \frac{3 \cdot 2^{2/3}}{5^{5/3}mc_0^{2/3}}n(x)^{5/3} - \frac{4}{45} \frac{2c_1 - 9c_2}{mc_0} \frac{(\nabla n(x))^2}{n(x)} - \frac{12}{5} \frac{c_2}{mc_0} \nabla^2 n(x). \quad (13)$$

The first two terms correspond to the local density approximation (LDA) and the terms proportional to c_1 and c_2 are the leading correction to the LDA involving derivatives of the density. We note that the last term proportional to $\nabla^2 n(x)$ does not contribute to the total energy of a finite system.

III. EPSILON EXPANSION

A. Lagrangian and Feynman rules

At unitarity the determination of c_1 and c_2 is a non-perturbative problem, and we will perform the calculation using an expansion around $d = 4 - \varepsilon$ spatial dimensions [11, 12]. The epsilon expansion has proven to be useful in calculating the equation of state [13], the critical temperature [14], few-body scattering observables [15], and the phase structure of spin-polarized systems [16]. Our starting point is the lagrangian

$$\mathcal{L} = \Psi^\dagger \left[i\partial_0 + \sigma_3 \frac{\vec{\nabla}^2}{2m} \right] \Psi + \mu \Psi^\dagger \sigma_3 \Psi + \left(\Psi^\dagger \sigma_+ \Psi \phi + h.c. \right) - \frac{1}{C_0} \phi^\dagger \phi, \quad (14)$$

where $\Psi = (\psi_\uparrow, \psi_\downarrow)^T$ is a two-component Nambu-Gorkov field, σ_i are Pauli matrices acting in the Nambu-Gorkov space, $\sigma_\pm = (\sigma_1 \pm i\sigma_2)/2$, ϕ is a complex boson field, and C_0 is a coupling constant. In dimensional regularization the fermion-fermion scattering length becomes infinite for $1/C_0 \rightarrow 0$.

The epsilon expansion is based on the observation that the fermion-fermion scattering amplitude near $d = 4$ dimensions is saturated by the propagator of a boson with mass $2m$. The coupling of the boson to pairs of fermions is given by

$$g = \frac{\sqrt{8\pi^2\varepsilon}}{m} \left(\frac{m\phi_0}{2\pi} \right)^{\varepsilon/4}. \quad (15)$$

In the superfluid phase ϕ acquires an expectation value $\phi_0 = \langle \phi \rangle$. We write the boson field as $\phi = \phi_0 + g\varphi$. The lagrangian is split into a free part

$$\mathcal{L}_0 = \Psi^\dagger \left[i\partial_0 + \sigma_3 \frac{\vec{\nabla}^2}{2m} + \phi_0(\sigma_+ + \sigma_-) \right] \Psi + \varphi^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \varphi, \quad (16)$$

and an interacting part $\mathcal{L}_I + \mathcal{L}_{ct}$, where

$$\mathcal{L}_I = g \left(\Psi^\dagger \sigma_+ \Psi \phi + h.c \right) + \mu \Psi^\dagger \sigma_3 \Psi + 2\mu \phi^\dagger \phi, \quad (17)$$

$$\mathcal{L}_{ct} = -\phi^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \phi - 2\mu \phi^\dagger \phi. \quad (18)$$

Note that the leading self energy corrections to the boson propagator generated by the interaction term \mathcal{L}_I cancel against the counterterms in \mathcal{L}_{ct} . The chemical potential term for the fermions is included in \mathcal{L}_I rather than in \mathcal{L}_0 . This is motivated by the fact that near $d = 4$ the system reduces to a non-interacting Bose gas and $\mu \rightarrow 0$. We will count μ as a quantity of $O(\epsilon)$. The Feynman rules are quite simple. The fermion and boson propagators are

$$G(p_0, p) = \frac{i}{p_0^2 - E_p^2} \begin{bmatrix} p_0 + \epsilon_p & -\phi_0 \\ -\phi_0 & p_0 - \epsilon_p \end{bmatrix}, \quad (19)$$

$$D(p_0, p) = \frac{i}{p_0 - \epsilon_p/2}, \quad (20)$$

where $E_p^2 = \epsilon_p^2 + \phi_0^2$ and $\epsilon_p = p^2/(2m)$. The fermion-boson vertices are $ig\sigma^\pm$. Insertions of the chemical potential are $i\mu\sigma_3$. Both g^2 and μ are corrections of order ϵ .

We shall make use of the following results that have been obtained at NLO in the epsilon expansion [12]

$$\phi_0 = \frac{2\mu}{\epsilon} \left[1 + (3C - 1 + \log(2))\epsilon + O(\epsilon^2) \right], \quad (21)$$

$$n = \frac{1}{\epsilon} \left[1 - \frac{1}{4}(2\gamma - 1 - 2\log(2)) + O(\epsilon^2) \right] \left(\frac{m\phi_0}{2\pi} \right)^{d/2}, \quad (22)$$

$$\xi = \frac{\epsilon^{3/2}}{2} \left[1 + \frac{1}{8}\epsilon \log(\epsilon) - \frac{1}{4}(12C - 5 + 5\log(2))\epsilon + O(\epsilon^2) \right]. \quad (23)$$

Here, ϕ_0 is the expectation value of the boson field, n is the density, and ξ determines the chemical potential in units of the Fermi energy, $\mu = \xi\epsilon_F$. The quantity $C \simeq 0.14424$ is a numerical constant that appears in the calculation of the two-loop effective potential, and $\gamma \simeq 0.57722$ is the Euler constant.

B. Phonon propagator

The phonon dispersion relation at LO in the epsilon expansion was obtained by Nishida in [14]. Here, we briefly review his results. We introduce a two-component scalar field $\Phi = (\phi, \phi^*)$. The

$$\left(\begin{array}{cc} \text{---} \rightarrow \text{---} & \leftarrow \text{---} \rightarrow \\ \text{---} \rightarrow \leftarrow \text{---} & \text{---} \leftarrow \text{---} \end{array} \right)^{-1} = \left(\begin{array}{cc} \text{---} \rightarrow \text{---} & \\ & \text{---} \leftarrow \text{---} \end{array} \right)^{-1} - \Pi$$

FIG. 1: Dyson Schwinger equation for the phonon propagator. Dashed lines denote the free boson propagator, double dashed lines denote the full propagator and Π is the boson self energy. Arrows show the order in which ϕ and ϕ^* are contracted.

scalar propagator is

$$\mathcal{D}^{-1}(p) = \mathcal{D}_0^{-1}(p) - \Pi(p) = \begin{pmatrix} [\mathcal{D}^{-1}(p)]_{11} & [\mathcal{D}^{-1}(p)]_{12} \\ [\mathcal{D}^{-1}(p)]_{21} & [\mathcal{D}^{-1}(p)]_{22} \end{pmatrix}, \quad (24)$$

where \mathcal{D} is the full propagator, \mathcal{D}_0 is the free propagator, and Π is the self energy, see Fig. 1. The free propagator does not have off-diagonal (anomalous) components. The diagonal terms are

$$[\mathcal{D}_0^{-1}(p)]_{11} = [\mathcal{D}_0^{-1}(-p)]_{22} = p_0 - \frac{\epsilon_p}{2}. \quad (25)$$

The self energy diagram at LO in the epsilon expansion are shown in Fig. 2. We find

$$\Pi_{11} = \Pi_{22} = -2\mu + \frac{3\epsilon\phi_0}{2} + O(\epsilon^2), \quad (26)$$

$$\Pi_{12} = \Pi_{21} = \frac{\epsilon\phi_0}{2} + O(\epsilon^2). \quad (27)$$

At leading order $\mu = \epsilon\phi_0/2$ and

$$\mathcal{D}(p) = \frac{1}{p_0^2 - \frac{\epsilon_p}{2}(\frac{\epsilon_p}{2} + 2\mu)} \begin{pmatrix} p_0 + \frac{\epsilon_p}{2} + \mu & -\mu \\ -\mu & -p_0 + \frac{\epsilon_p}{2} + \mu \end{pmatrix}. \quad (28)$$

The dispersion relation is

$$p_0 = \frac{1}{2} \sqrt{\epsilon_p(\epsilon_p + 4\mu)} \simeq \sqrt{\mu\epsilon_p} \left(1 + \frac{\epsilon_p}{8\mu} + \dots \right), \quad (29)$$

which shows that the spectrum contains a Goldstone mode with a linear dispersion relation, $p_0 \simeq v_s p$, where $v_s = \sqrt{\mu/(2m)}$.

$$-\Pi = \begin{pmatrix} \text{---}\times\text{---} & \text{---}\rightarrow\bullet\rightarrow\text{---} & \text{---}\rightarrow\bullet\rightarrow\text{---} \\ \text{---}\leftarrow\bullet\leftarrow\text{---} & \text{---}\times\text{---} & \text{---}\leftarrow\bullet\leftarrow\text{---} \end{pmatrix}$$

FIG. 2: Leading order contributions to the boson self energy. Full lines denote fermion propagators in the Nambu-Gorkov representation. Arrows indicate the order in which Ψ and Ψ^\dagger are contracted. A cross denotes a μ -insertion from \mathcal{L}_I . There is a contribution from the first counterterm in \mathcal{L}_{ct} which is not shown here.

C. Static susceptibility

The one-loop contribution to the static susceptibility (see Fig. 3a) is

$$\begin{aligned} \chi(q) &= -i \int \frac{d^d k}{(2\pi)^d} \int \frac{dk_0}{2\pi} \text{Tr}[G(k+q/2)\sigma_3 G(k-q/2)\sigma_3] \\ &= -\frac{1}{\phi_0} \left\{ 1 - \frac{1}{2}(\gamma - 1 + \log(2))\epsilon - \frac{1}{12} \left(\frac{q^2}{m\phi_0} \right) + O(\epsilon^2) \right\} \left(\frac{m\phi_0}{2\pi} \right)^{d/2}, \end{aligned} \quad (30)$$

where we have expanded $\chi(q)$ in powers of momentum, treating q^2 as a quantity of order ϵ . We observe that the one-loop contribution scales as $\chi(0) \sim \epsilon^0$. This should be compared to the thermodynamic result $\chi(0) = -(\partial n)/(\partial \mu) \sim \epsilon^{-2}$. In order to get an enhancement by two inverse powers of ϵ we need to consider graphs that contain massless particles. The dominant contribution comes from phonons, see Fig. 3b,c. The LO phonon term is

$$\chi(q) = g^2 \left\{ \Pi_{3+}(q) \mathcal{D}_{11}(q) \Pi_{3-}(q) + \Pi_{3+}(q) \mathcal{D}_{12}(q) \Pi_{3+}(q) + h.c. \right\} \quad (31)$$

where \mathcal{D}_{ij} is the phonon propagator and

$$\begin{aligned} \Pi_{3\pm}(q) &= -i \int \frac{d^d k}{(2\pi)^d} \int \frac{dk_0}{2\pi} \text{Tr}[G(k+q/2)\sigma_3 G(k-q/2)\sigma_{\pm}] \\ &= -\frac{1}{\epsilon\phi_0} \left\{ 1 - \frac{1}{2}(\gamma - \log(2))\epsilon + \frac{1}{8}(\gamma - \log(2))^2 \epsilon^2 - \frac{1}{24} \left(\frac{q^2}{m\phi_0} \right) \epsilon \right\} \left(\frac{m\phi_0}{2\pi} \right)^{d/2} \end{aligned} \quad (32)$$

Using the leading order phonon propagator derived in the previous section we find in the static limit

$$\mathcal{D}_{11}(q) + \mathcal{D}_{12}(q) = -\frac{1}{2\mu + \epsilon q/2} = -\frac{1}{2\mu} \left\{ 1 - \frac{1}{8} \left(\frac{q^2}{m\mu} \right) + O(q^4) \right\} \quad (33)$$

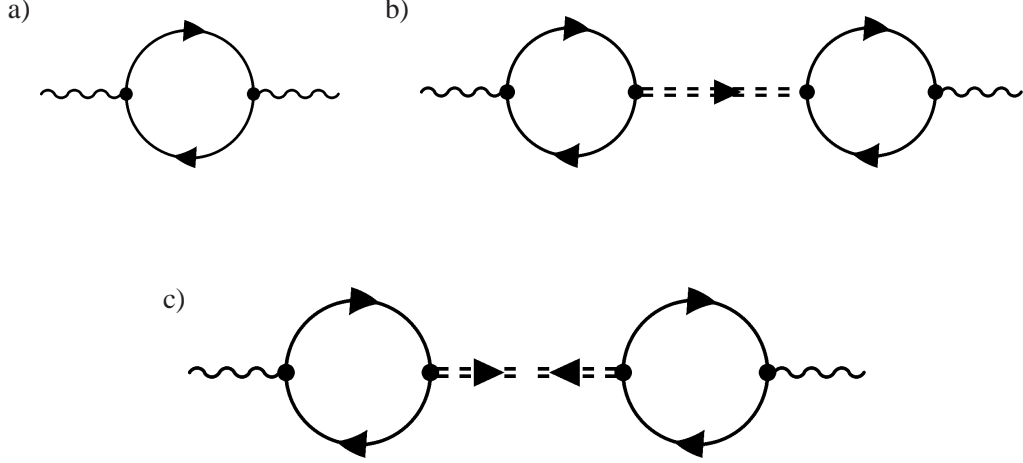


FIG. 3: Fig. a) shows the one-loop contribution to the static susceptibility. The wavy line denotes an external source coupled to $\psi^\dagger\psi$. Figs. b) and c) show the leading order phonon contribution. The double dashed line is full phonon propagator defined in Fig. 1.

We can now determine the static susceptibility

$$\chi(q) = -\frac{2}{\epsilon\mu} \left[1 - (\gamma - \log(2))\epsilon + O(\epsilon^2) \right] \left\{ 1 - \frac{1}{8} \left(\frac{q^2}{m\mu} \right) + O(q^4) \right\} \left(\frac{m\phi_0}{2\pi} \right)^{d/2}. \quad (34)$$

We can compare the momentum independent term to the prediction from the relation $\chi(0) = -(\partial n)/(\partial \mu)$. Using equ. (22) and (21) we find, at NLO in the ϵ expansion,

$$\chi(0) = -\frac{2}{\epsilon\mu} \left\{ 1 - \frac{1}{2} (\gamma - \log(2))\epsilon + O(\epsilon^2) \right\} \left(\frac{m\phi_0}{2\pi} \right)^{d/2}. \quad (35)$$

which agrees at leading order, but not at NLO.

D. Higher order corrections

The LO phonon dispersion relation and susceptibility depend on $O(\epsilon)$ terms in the boson self energy. The NLO phonon dispersion relation requires $O(\epsilon^2)$ corrections. Since the LO curvature term in the dispersion relation is proportional to $p^2/(m\mu)$ we can count p_0, ϵ_p as quantities of order ϵ . The one-loop self energies, expanded to NLO in ϵ , are given by

$$\Pi_{11} = -\left(p_0 - \frac{\epsilon_p}{2}\right) \left\{ 1 - \frac{1}{2} (\gamma - \log(2))\epsilon \right\} + \frac{3\epsilon\phi_0}{2} \left\{ 1 + \frac{1}{6} (5 - 3\gamma - \log(8))\epsilon \right\} + \dots \quad (36)$$

$$\Pi_{12} = \frac{\epsilon\phi_0}{2} \left\{ 1 + \frac{1}{2} (1 - \gamma - \log(2))\epsilon \right\} - \frac{\epsilon\epsilon_p}{8} + \dots \quad (37)$$

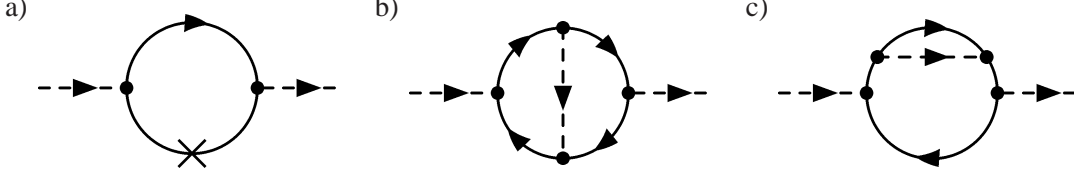


FIG. 4: Higher order contributions to the diagonal boson self energy Π_{11} . Fig. a) shows a μ -insertion into the one-loop self energy. This diagram is combined with the second counterterm from \mathcal{L}_{ct} (not shown). Figs. b) and c) show the “vertex-type” and “self energy-type” two-loop contributions. The corresponding contributions to the off-diagonal self energy Π_{12} are not shown.

and the NLO expression for ϕ_0 is given in equ. (21). The term $-(p_0 - \epsilon_p/2)$ is canceled by the first counterterm in \mathcal{L}_{ct} . The μ insertion into the one-loop self energy is

$$\Pi_{11} = -2\mu \left\{ 1 - \frac{1}{4}(1 + 2\gamma - 2\log(2))\epsilon + O(\epsilon^2) \right\} \quad (38)$$

$$\Pi_{12} = \frac{\mu\epsilon}{2} \left\{ 1 + O(\epsilon) \right\}, \quad (39)$$

where the term -2μ is canceled by the second counterterm in \mathcal{L}_{ct} . There are two two-loop self energy diagrams, see Fig. 4. We will compute these diagrams in App. A. The result can be written as

$$\Pi_{11} = C_1 \phi_0 \epsilon^2, \quad \Pi_{12} = C_2 \phi_0 \epsilon^2, \quad (40)$$

where $C_{1,2}$ are numerical constants. These two constants are constrained by some general relations. First, the phonon is a Goldstone mode and the dispersion relation has to satisfy $\omega_q(q=0) = 0$. We also know that the velocity of sound is related to the equation of state. In $d = 4 - \epsilon$ dimensions

$$v_s = \sqrt{\frac{\xi}{d}} v_F = \sqrt{\frac{\mu}{2m}} \left(1 + \frac{\epsilon}{8} + O(\epsilon^2) \right). \quad (41)$$

These two conditions determine $C_{1,2}$. We find

$$C_1 = -\frac{9}{2}C \simeq -0.64908, \quad C_2 = -\frac{3}{2}C \simeq -0.21636. \quad (42)$$

In App. A we demonstrate that these results agree with an explicit calculation of the two-loop self energies. With these results, the inverse boson propagator at NLO takes on a very simple form.

We find

$$\mathcal{D}^{-1} = Z \begin{pmatrix} p_0 - \frac{\epsilon_p}{2} - \mu & \frac{\epsilon\epsilon_p}{8} - \mu \\ \frac{\epsilon\epsilon_p}{8} - \mu & -p_0 - \frac{\epsilon_p}{2} - \mu \end{pmatrix}, \quad Z = 1 - \frac{1}{2}(\gamma - \log(2))\epsilon \quad (43)$$

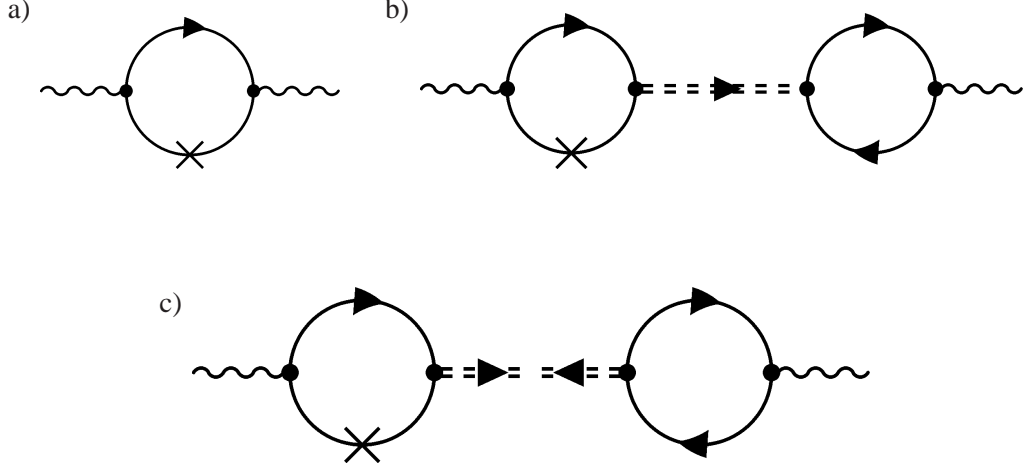


FIG. 5: Higher order contributions to the static susceptibility. Fig. a) shows the μ -insertion into the one-loop diagram, Figs. b) and c) show μ -insertions into the phonon contribution.

The phonon dispersion relation is

$$p_0 = \sqrt{\mu \epsilon_p} \left(1 + \frac{\epsilon}{8} \right) \left\{ 1 + \frac{\epsilon_p}{8\mu} \left(1 - \frac{\epsilon}{4} \right) + \dots \right\} \quad (44)$$

We now consider NLO corrections to the static susceptibility, see Fig. 5. The first diagram is the μ -insertion into the one-loop graph. This graph is $O(\epsilon\mu)$, which is an $O(\epsilon^4)$ correction to the leading order term in $\chi(0)$. The second and third diagram contain μ -insertions into Π_{3+} . These diagrams are $O(1)$, an $O(\epsilon^2)$ correction to the leading term. Two-loop corrections to Π_{3+} are also suppressed by at least two powers of ϵ . This means that, in addition to NLO corrections from the one-loop Π_{3+} already given in equ. (34), NLO corrections to the static susceptibility arise solely from higher order corrections to the boson propagator. We find

$$\chi(q) = -\frac{2}{\epsilon\mu} \left[1 - \frac{1}{2} (\gamma - \log(2)) \epsilon \right] \left\{ 1 - \frac{1}{8} \left(\frac{q^2}{m\mu} \right) \left(1 - \frac{\epsilon}{4} \right) + O(q^4) \right\} \left(\frac{m\phi_0}{2\pi} \right)^{d/2}. \quad (45)$$

We observe that $\chi(0)$ matches the NLO prediction from the relation $\chi(0) = -(\partial n)/(\partial \mu)$, see equ. (35).

IV. MATCHING

We found that the leading terms in a small momentum expansion of the phonon dispersion relation and the static susceptibility satisfy the low energy predictions $v_s^2 = (\partial P)/(\partial \rho)$ and $\chi(0) =$

$-(\partial n)/(\partial \mu)$ at NLO in the epsilon expansion. This means that we can use the curvature terms to fix the low energy constants c_1 and c_2 . In order to be consistent with the low energy theorems we have to perform the matching in $d = 4 - \epsilon$ dimensions. The low energy effective Lagrangian in d dimensions is

$$\mathcal{L} = c_0 m^{d/2} X^{1+d/2} + c_1 m^{d/2-1} \frac{(\vec{\nabla} X)^2}{X^{2-d/2}} + \frac{c_2}{m^{2-d/2}} \left[(\nabla^2 \phi)^2 - d^2 m \nabla^2 V \right] X^{d/2-1}. \quad (46)$$

The powers of m and X follow from the scaling dimension of the fields. The factor d^2 in the c_2 -term is a non-trivial consequence of conformal invariance in d dimensions [10]. In d dimensions the relation between c_0 and $\xi = \mu/\epsilon_F$ is

$$c_0 = \frac{2}{(2\pi)^{d/2} \Gamma(2 + d/2) \xi^{d/2}}. \quad (47)$$

The two NLO parameters c_1, c_2 can be related to the momentum dependence of the phonon dispersion relation and the static susceptibility. In d dimensions we find

$$q_0 = v_s q \left[1 - \frac{4}{d(d+2)c_0} \left(c_1 + \frac{d}{2} c_2 \right) \frac{q^2}{m\mu} \right] \quad (48)$$

and

$$\chi(q) = -\frac{d(d+2)c_0}{4} m^{d/2} \mu^{d/2-1} \left[1 + \frac{8}{d(d+2)c_0} \left(c_1 - d^2 \left(\frac{d}{2} - 1 \right) c_2 \right) \frac{q^2}{m\mu} \right]. \quad (49)$$

We can now match the curvature terms in equ. (44) and (45) to equ. (48) and (49). From the phonon dispersion relation we get

$$c_1 + \frac{d}{2} c_2 = -\frac{d(d+2)c_0}{64} \left(1 - \frac{\epsilon}{4} \right). \quad (50)$$

Matching the static susceptibility gives

$$c_1 + \frac{d}{2} c_2 = c_1 - d^2 \left(\frac{d}{2} - 1 \right) c_2. \quad (51)$$

This implies that c_2 vanishes to NLO in the epsilon expansion $c_2/c_1 = O(\epsilon^2)$. This is (barely) consistent with the constraint $c_2 > 0$ [10]. The ratio c_1/c_0 is given by

$$\frac{c_1}{c_0} = -\frac{3}{8} \left(1 - \frac{2\epsilon}{3} + \dots \right). \quad (52)$$

At NLO we obtain the following density functional for non-relativistic fermions at infinite scattering length

$$\mathcal{E}(x) = n(x)V(x) + 1.364 \frac{n(x)^{5/3}}{m} + 0.022 \frac{(\nabla n(x))^2}{mn(x)} + O(\nabla^4 n). \quad (53)$$

It is interesting to compare this result to the density functional for non-interacting fermions [17]

$$\mathcal{E}_{ETF}(x) = n(x)V(x) + 2.871 \frac{n(x)^{5/3}}{m} + 0.014 \frac{(\nabla n(x))^2}{mn(x)} + 0.167 \frac{\nabla^2 n(x)}{m} + O(\nabla^4 n), \quad (54)$$

which is known as the “extended Thomas-Fermi model” (ETF). The energy of N fermions in a spherically symmetric harmonic trap is

$$E = \frac{\sqrt{\xi}}{4} \omega (3N)^{4/3} \left(1 + \frac{c_s}{(3N)^{2/3}} + \dots \right), \quad (55)$$

where $\xi \simeq 0.475$ (see equ. (23)) and $c_s = -(32c_1)/(5c_0\xi) \simeq 1.68$ at NLO in the epsilon expansion. The result for free fermions is

$$E_{ETF} = \frac{1}{4} \omega (3N)^{4/3} \left(1 + \frac{1}{2(3N)^{2/3}} + \dots \right), \quad (56)$$

We observe that the coefficient of the $N^{4/3}$ term in the ETF functional is larger than the corresponding coefficient in the unitarity limit. This simply reflects the fact that the interaction between the fermions is attractive and $\xi < 1$. What is more surprising is the fact that the ETF functional corresponds to a significantly smaller value of c_s . Numerical results for up to $N = 30$ harmonically trapped fermions can be found in [18, 19, 20]. For small N the corrections to the local density approximation are not very well fit by a $N^{-2/3}$ contribution, and the authors of [18, 19] did not attempt to extract ξ and c_s independently. Under the assumption that the data can be described by $E = \xi E_{ETF}$ they find values $\xi \simeq (0.47 - 0.50)$ which are larger than the commonly accepted bulk value $\xi \simeq (0.40 - 0.44)$ [21, 22, 23, 24]. On the other hand, accepting the bulk value $\xi = (0.40 - 0.44)$ implies larger values of c_s than the one predicted by the extended Thomas-Fermi model. Taking $E(N = 20) = (41.3 - 43.2)\omega$ from [18, 19] and $\xi = (0.40 - 0.44)$ gives $c_s = (0.9 - 2.5)$, consistent with our result $c_s = 1.68$. We note that the data of [18, 19, 20] are even better fit by a functional of the form $E(N) = \omega \sqrt{\xi}/4 \cdot (3N)^{4/3} (1 + c/(3N)^{1/3})$. A correction of the form $1/N^{1/3}$ cannot be obtained from a local energy density functional of the form given in equ. (13), nor is it compatible with the structure of non-leading terms in N generally assumed in the literature [25, 26]. It is an interesting challenge to determine whether more complicated functionals (see Sec. V) can yield corrections to the energy of N harmonically trapped fermions that scale as $1/N^{1/3}$.

V. SUMMARY AND OUTLOOK

We have computed an energy density functional for dilute non-relativistic fermions at unitarity. Our approach is based on an effective field theory of the unitary gas which takes into account the effects of spontaneous symmetry breaking, the existence of Goldstone modes, and the constraints from Galilean and conformal symmetry. We have used an epsilon expansion to compute the coefficients in the effective lagrangian at NLO in the derivative expansion. Our main result is given in equ. (53). It is interesting that at NLO in the epsilon expansion only one of the two possible two-derivative terms appears.

There are several interesting lines of investigation that we wish to pursue in the future. The first is the problem of constructing energy density functionals that depend on more than one type of density. One may consider, for example, the spin density (mostly of interest for applications in atomic physics), or the superfluid density [27, 28, 29, 30]. It is also important to find a systematic way of constructing functionals of the Kohn-Sham type [31, 32], or extensions of Kohn-Sham theory that contain anomalous densities (as in the Hartree-Fock-Bogoliubov approximation), see [27]. Finally, it is important to study more realistic interactions for neutron matter, in particular the effects of a finite scattering length or non-zero effective range [33], and the effects of explicit pion degrees of freedom

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APPENDIX A: TWO-LOOP SELF ENERGY DIAGRAMS

In the appendix we compute the two-loop self energy diagrams that contribute to the phonon propagator at NLO. The two-loop “vertex-type” diagram shown in Fig. 4b) is given by

$$\begin{aligned}
-i\Pi_{11}^{(b)}(p) &= -g^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{dq_0}{2\pi} \frac{dk_0}{2\pi} [G_{11}(k)G_{21}(q)G_{22}(q-p)G_{12}(k-p)D(k-q) \\
&\quad + G_{12}(k)G_{11}(q)G_{21}(q-p)G_{22}(k-p)D(q-k)], \\
-i\Pi_{21}^{(b)}(p) &= -g^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{dq_0}{2\pi} \frac{dk_0}{2\pi} [G_{12}(k)G_{12}(q)G_{22}(q-p)G_{11}(k-p)D(k-q) \\
&\quad + G_{22}(k)G_{11}(q)G_{12}(q-p)G_{12}(k-p)D(q-k)].
\end{aligned} \tag{A1}$$

In the ϵ -expansion, counting $p_0 \sim p^2 \sim \epsilon$ we only need the self-energy correction at zero energy and momentum. We get

$$\begin{aligned}
-i\Pi_{11}^{(b)}(0) &= -i\Pi_{21}^{(b)}(0) \\
&= -ig^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{\partial}{\partial q_0} \frac{\partial}{\partial k_0} \left[\frac{k_0 + \epsilon_k}{(k_0 - E_k)^2} \frac{q_0 - \epsilon_k}{(q_0 - E_q)^2} \frac{1}{k_0 - q_0 - \epsilon_{q-k}/2} \right] \Big|_{\substack{q_0 \rightarrow E_q \\ k_0 \rightarrow -E_k}} \\
&= -i \frac{4\phi_0 \epsilon^2}{\pi} a + O(\epsilon^3).
\end{aligned} \tag{A2}$$

The constant a can be determined by performing the integrals in $d = 4$ spatial dimensions. A numerical calculation gives $a \simeq -0.267359$.

The “self energy-type” two-loop Feynman diagram Fig. 4c) is given by

$$\begin{aligned}
-i\Pi_{11}^{(c)} &= -2g^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{dq_0}{2\pi} \frac{dk_0}{2\pi} [G_{11}(k)G_{11}(k)G_{22}(q)G_{22}(k-p)D(k-q) \\
&\quad + G_{11}(q)G_{12}(k)G_{21}(k)G_{22}(k-p)D(q-k)] \equiv B + F, \\
-i\Pi_{21}^{(c)} &= -2g^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{dq_0}{2\pi} \frac{dk_0}{2\pi} [G_{11}(k)G_{21}(k)G_{21}(k-p)G_{22}(q)D(k-q) \\
&\quad + G_{22}(k)G_{21}(k)G_{21}(k-p)G_{11}(q)D(q-k)] \equiv H + K.
\end{aligned} \tag{A3}$$

In the limit $p = 0$, changing variables $k_0 \rightarrow -k_0$ shows that $F = K$ and $F = H$. We get

$$\begin{aligned}
B &= -ig^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{E_q - \epsilon_q}{2E_q} \frac{\partial^2}{\partial k_0^2} \left[\frac{(k_0 + \epsilon_k)^2 (k_0 - \epsilon_k)}{(k_0 - E_k)^3 (k_0 - E_q - \epsilon_{k-q}/2)} \right] \Big|_{k_0 = -E_k} \\
&\equiv -i \frac{2\phi_0 \epsilon^2}{\pi} b, \\
F &= -ig^4 \int \frac{dq^d}{(2\pi)^d} \frac{dk^d}{(2\pi)^d} \frac{E_q - \epsilon_q}{2E_q} \frac{\partial^2}{\partial k_0^2} \left[\frac{(k_0 - \epsilon_k) \phi_0^2}{(k_0 + E_k)^3 (-k_0 - E_q - \epsilon_{k-q}/2)} \right] \Big|_{k_0 = E_k} \\
&\equiv -i \frac{2\phi_0 \epsilon^2}{\pi} f.
\end{aligned} \tag{A4}$$

Numerical evaluation gives $b \simeq -0.5822930$ and $f = h = k \simeq 0.09742858$. Collecting all the terms

$$\begin{aligned}
\Pi_{11}^{(b)}(0) + \Pi_{11}^{(c)}(0) &= \frac{2\phi_0 \epsilon^2}{\pi} (2a + b + f) = C_1 \phi_0 \epsilon^2 \simeq -0.64908 \phi_0 \epsilon^2, \\
\Pi_{21}^{(b)}(0) + \Pi_{21}^{(c)}(0) &= \frac{4\phi_0 \epsilon^2}{\pi} (a + f) = C_2 \phi_0 \epsilon^2 \simeq -0.21636 \phi_0 \epsilon^2,
\end{aligned} \tag{A5}$$

which agree very well with the determination in equ. (42).

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